Summaries

UDC 546.72:544.778.4:66.094.3-926-217:543.573

Korshunov A.V.
THE INFLUENCE OF IRON POWDER DISPERSITY ON LAWS OF THEIR OXIDATION AT HEATING IN THE AIR

The laws of oxidation process of industrial micron powder and electro blasting iron nanopowder at heating in the air under conditions of linearly increasing temperature and isothermal mode have been studied. Oxidation process staging in conditions of linear heating conditioned by total influence of powder fractional composition and phase composition and structure of the oxide layer formed on particle surface was shown. It was shown that nanopowder oxidation process in comparison with micron powder in isothermal conditions (250...600 °C) was described by linear law and occurred in kinetic mode (E_a=100±7 kJ/mole). The conditions of thermogravimetry at which nanopowder thermal self-ignition occurs were determined; the experimentally fixed value of critical temperature was substantiated on the basis of numerical estimation of sample surface heating parameter.

UDC 546.59:547.477.1:544.773.422

Korshunov A.V., Kashkan G.V., Nguen Kh.T.T., Zyong Sh.V.
KINETICS OF FORMING PARTICLES OF GOLD SOL DISPERSION PHASE

Kinetic laws of forming gold sol without high molecular stabilizers using sodium citrate as deoxidant have been studied. The range of agents $HAuCl_4$ and $Na_3C_6H_5O_7$ concentration, pH interval and the values of solution ionic strength, at which stable sol is formed spontaneously without heating the reaction mixture, were ascertained. Reagent local orders and effective activation energy of growth process of Au (42±3 kJ/mole) particles were determined. It was shown that the process of forming dispersion phase particles in the test system is not coordinated with the model of homogeneous nucleation. The explanation of stages of forming sol particles occurring with colloid intermediates of Au (III) and Au (I) hydroxides (oxides) fulfilling a function of centers of nucleation and next growth of metal parts was proposed.

UDC 544.5

Radishevskaya N.I., Chapskaya A.Yu., Lvov O.V., Vereschagin V.I., Korshunov A.V.
COMPOSITION AND STRUCTURE OF PROTECTION OXIDE-HYDROXIDE COVER ON ALUMINUM NANOP OWDER PARTICLES

It was ascertained that the structure of hydroxide phases in composition of surface layer of aluminum nanopowder particles depends on passivation conditions, conditions and duration of storage, size of aluminum nanopowder particles and admixture occurrence. It was shown that thermal treatment of aluminum nanopowders to 550 °C results in formation of oxide γ-Al_2O_3 particles on the surface. The diagram of forming hydrox-oxide layer on aluminum surface was introduced.

UDC 544.45

Ilyin A.P., Root L.O., Zvyagintseva E.S.
METHODS OF INCREASING NITRIDE YIELD IN AIR COMBUSTION PRODUCTS OF ALUMINUM NANOPOWDERS AND ITS MIXTURES

The experimental techniques of increasing aluminum nitride yield after aluminum nanopowder combustion in the air: increasing mass of aluminum nanopowder, restriction of air volume etc have been considered. The influence of IR radiation on burnt samples of aluminum nanopowders and its mixtures on aluminum and titanium nitrides yield was experimentally studied. An ambiguous influence of radiation on nitride yield was determined.

UDC 542.06;544.77

Machekhina K.I., Shiyan L.N., Tropina E.A., Klupfel A.
STUDYING THE PROCESSES OF ULTRA- AND NANO-FILTRATION OF COLLOIDAL IRON SOLUTIONS

The processes of ultra- and nano-filtration of colloidal solutions containing soluble organic substances and ions of iron and silicon have been studied using a membrane module. It was ascertained that the use of ultra-filtration membrane GR81PP is appropriable for natural waters without silicon ions and for waters containing silicon ions it is appropriable to use NF90 and NF270 nano-filtration membranes. The membrane selectivity magnitudes relative to ions of iron, silicon and organic substance were calculated. The processes of ultra- and nano-filtration are supposed to be used as a stage of polishing treatment for ground waters of Western Siberia.

UDC 666.291.3

Sedelnikova M.B., Liseenko N.V., Pogrebenkov V.M.
CERAMIC PIGMENTS WITH DIORTOSILICATE STRUCTURE

The synthetic processes of ceramic pigments with diortosilicate structures – helenite, hardystonite, akermanite have been studied using natural wollastonite and nepheline slime. It was ascertained that synthetic reactions run more successfully in the temperature range 1100...1200 °C with nepheline slime than with wollastonite but the presence of iron oxide in nepheline slime affects negatively on color properties of cobalt- and nickel bearing pigments.

UDC 546.791;661.66.074.3;661.48

Gromov O.B., Djyachenko A.N., Petrov D.A., Seredenko V.A.
TUNGSTEN AND MOLYBDENUM EJECTION FROM URANIUM-BEARING SOLUTIONS OF RECOVERY SYSTEM OF SUBLIMATE PRODUCTION WASTES

It was shown that composition of back U_3O_8 obtained in uranium recovery system from sublimate production wastes influences considerably on quality of uranium hexafluoride. The process of sorption purification of uranium sulfate-fluoride solutions from tungsten and molybdenum admixtures using inorganic sorbent «Thermoxide-5»

was studied. It was shown that addition of aluminum sol into solution does not affect the solution purification but prevents dissolution of sorbent base. The data for improving the diagram of uranium recovery form liquid wastes of sublimate production were obtained.

UDC 51-73

Krivtsov P.Yu., Pavlov V.M.
DEVELOPING THE MODEL OF CHEMICAL REACTOR OF THE UNIT FOR PROCESSING SODIUM COOLANT

Quantitative characteristics of material flows of the basic components and reaction products have been obtained; the rate of process behavior at different initial conditions has been studied. Mathematical description of chemical process was given; physical properties of components were determined in the form of analytic dependences. Modeling researches of chemical reactor of the unit for sodium processing were carried out.

UDC 543.063

Slepchenko G.B., Gindullina T.M., Cherempey E.G., Khlusov I.A., Schukina T.I., Feduschak T.A.
DEVELOPMENT OF VOLTAMMETERY DETERMINATION OF IRON AND SILVER FOR ESTIMATING NANO-PARTICLE DEGRADATION DEGREE ON THEIR BASIS

The issues of applying electrochemical methods for controlling nano-particle toxicity in biological objects have been considered. The possibility of using voltammetry method for determining ions of silver, iron and estimating the degradation degree of Fe_3O_4 nano-particles was shown for the first time.

UDC 546.15:543.253

Moskaleva M.L., Noskova G.N., Kolpakova N.A.
DETERMINING NITRITE BY THE METHOD OF VOLTAMMETRY AT GOLD MICROELECTRODE ARRAY

The technique of determining nitrite by the method of direct voltammetry applying the gold microelectrode array on the basis of carbon composite solid electrode has been proposed. Optimal conditions of preparing microelectrode array were selected. The influence of base solution composition and parameters of voltamperogramm recording on analytic signal of nitrite was studied. The technique of determining nitrite in drinking and low-mineralized natural waters was developed on the basis of the proposed method.

UDC 543.522;543.08

Larionova E.V., Diaz-Cruz H.M., Romanenko S.V.
MODIFICATION OF THE METHOD OF MULTIVARIATE RESOLUTION OF VOLTAMMETRY DATA

The algorithm of multivariate resolution of voltammetry data has been modified with optimization by the changing least square method using the efficient peak model. The peak model of voltammetry signal which is the logarithmic modification of abscissa of function of the derivative logista was selected on the basis of integrated system of classifying models of analytic signals in the form of peaks. Application of modified resolution algorithm when studying complex formation of zinc with glutathione by the method of differential-pulse polarography was shown.

UDC 543.552

Perevezentseva D.O., Chernyshova N.N.
SUPPORTING ELECTROLYTE AFTER DIRECT CURRENT ACTION IN VOLTAMPEROMETRIC ANALYSIS

The diagram of ascertaining cause-effect relations between the solution condition after direct current action in anode chamber of membrane cell and parameters of analytic signal of potential-defining element, its characteristic relations in voltammetry as well as the state of solution after direct current action in anode chamber of membrane cell has been proposed. The decrease of interfering influence of surface-active agent of cetyl pyridinium chloride after its addition into solution of supporting electrolyte after direct current action was shown. A new method of carrying out voltamperometric analysis of water tests based on using supporting electrolyte solution after direct current action was proposed.

UDC 543.552

Martynyuk O.A., Slepchenko G.B., Prikhodko V.A., Postnikov P.S., Trusova M.E.
POSSIBILITIES OF APPLYING NEW ORGANO-MODIFIED ELECTRODES IN QUALITY CONTROL OF JUICES AND NECTARS

Voltamperometric method of determining water-soluble vitamins on modified graphite electrodes has been developed. A new electrode organo-modified with aryldiazonium tosilate salts was proposed. The conditions of determining water-soluble vitamins are optimized and the technique for their quantitative chemical analysis using organo-modified electrodes in juice and nectar was developed. The correctness of the results was checked by «introduced-found» technique. The proposed technique of determining vitamins at modified electrodes allows increasing sensitivity in 3...4 times and decreasing the error of determination to 14...18 %.

UDC 661.721.41:544.478-03:544.18

Kravtsov A.V., Popok E.V., Yuriev E.M.
STUDYING THE MECHANISM OF CO CONSERVATION AT Zn-Cu-Al-CATALYST BY QUANTUM-THEORY METHODS

The principle approaches to considering CO adsorption mechanism at low-temperature Zn-Cu-Al catalysts of methanol synthesis have been studied. The analysis of synthesis mechanism considering formation of positively charged chemisorbed complex was carried out by quantum-theory methods. The structures of catalyst active centers were studied. Binding energies between the adsorbed CO molecule and catalyst active center were calculated.

UDC 66.097:667.6

Lymareva A.V., Fiterer E.P., Pokharukova Yu.E.
INVESTIGATION OF CATALYTIC OLIGOMERIZATION OF PYROLYSIS BY-PRODUCTS

The process of catalytic oligomerization of unsaturated compounds of C_9 fraction which is a by-product of «Angarsk polymer plant» manufacturing has been studied for obtaining film-forming oligomer. Physical and chemical properties of the obtained oligomers were studied.

UDC 665.633

Smyshlyaeva Yu.A., Ivanchina E.D., Kravtsov A.V., Zyong Ch.T., Fan F.
THE DEVELOPMENT OF OCTANE NUMBER DATABASE FOR MATHEMATICAL MODEL OF FINISHED GASOLINE COMPOUNDING PROCESS

A new approach to calculating the process of preparing gasoline using the mathematical modeling method has been stated. The aggregated database on octane numbers of fuel mixture components which may be used for calculation of octane numbers of finished gasoline mixing by computer modeling system was developed.

UDC 541.11

Frantsina E.V., Afanasieva Yu.I., Ivashkina E.N., Ivanchina E.D.
THERMODYNAMIC ANALYSIS OF DEHYDROGENATING PROCESS OF HIGHER PARAFFINS C_9–C_{14} WITH NORMAL STRUCTURE

The formalized scheme of substance conversion has been drawn on the basis of thermodynamic modeling of different types of reactions of dehydrogenating process of normal structure higher hydrocarbons C_9–C_{14}; the probability of their behavior has been estimated. Using the quantum-chemical calculations it was shown in what way the main thermodynamic characteristics of reactions change in conditions of industrial process.

UDC 541.64:667.6

Petukhova A.V., Ionova E.I., Lyapkov A.A., Petrenko T.V.
OLIGOMERIZATION OF C_9 FRACTION UNDER THE ACTION OF TRICHLORO(2-CHLORPROPOXY)TITANIUM IN TOLUENE SOLUTION

The kinetic of oligomerization process of C_9 fraction under the action of trichloro(2-chlorpropoxy)titanium has been studied by the method of adiabatic thermometry. The magnitudes of the observed constants of C_9 fraction oligomerization and heat release in the system were determined. The cover properties were analyzed on the basis of the obtained oligomers.

UDC 541.64:544.16

Bondaletov V.G., Bondaletov O.V., Bondaletova L.I., Bochkarev V.V.
STUDYING COMPLEXES OF ACRYL ETHERS WITH TITANIUM TETRACHLORIDE

The interaction of methyl-acrylic acid ethers with titanium tetrachloride results in formation of complexes capable of reacting with monomers of liquid pyrolysis products generating modified polymeric petroleum resins. The obtained complexes were studied using NMR ^{1}H-spectroscopy and semi-empirical method PM6.

UDC 541.64:547.759.32

Lyapkov A.A., Ionova E.I., Bondaletov V.G.
OLYGOMERIZATION OF α-METHYLSTYRENE UNDER THE ACTION OF CATALYSTS ON THE BASIS OF TITANIUM TETRACHLORIDE

The laws of olygomerization of α-methylstyrene under the action of catalysts on the basis of titanium tetrachloride in toluene solution have been studied using an adiabatic reactor. The effective values of chain growth rate constant both on pure titanium tetrachloride and on its complex with diethylaluminum chloride of composition 1:1 were calculated. It was shown that the presence of slower stage, during which the active center concentration may increase to steady state, conditions *S*-shaped form of kinetic curves. The obtained data may be used at modeling olygomerization of pyrolysis liquid products.

UDC 541.64:547.759.32

Ionova E.I., Lyapkov A.A., Bondaletov V.G.
PROCESSES OF OXIDATION AND STRUCTURING OF OLIGOMERS ON THE BASIS OF DICYCLOPENTADIENE

It was shown that oligomeric film coatings obtained from dicyclopentadiene or liquid products of pyrolysis containing dicyclopentadiene are subjected to oxidation and structuring in the air. Olefinic functionality is oxidized in films in the air smoothly during some weeks. This oxidation is accompanied by the growth of absorption band of carbonyl and hydroxyl groups in IR-spectra of oligomers. The process of oxidative thermal decomposition of oligomeric products on the basis of dicyclopentadiene is accompanied by extraction of low-molecular oxidation products.

UDC 547.281;547.284;547.572

Yusubov M.S., Galaktionova A.S., Tveryakova E.N., Perederina I.A., Drygunova L.A., Zykova M.V., Larkina M.S., Zholobova G.A., Korzh A.P., Smolyakov A.V., Funk T.V., Miroshnichenko Yu.Yu.
SYNTHESIS OF 4-IODINE AND 4-IODOSYLBENZENESULFONIC ACID

The methods of obtaining 4-iodosylbenzenesulfonic acid and 4-iodosylbenzenesulfonic acid as a reagent capable of recycle have been proposed. Preparative possibilities of this compound of polyvalent iodine are shown by the example of oxidation of secondary alcohols to ketones and α-methoxylation of ketones.

UDC 535.37:539.19:541.14

Ermolina E.G., Kuznetsova R.T., Solodova T.A., Kopylova T.N., Telminov E.N., Mayer G. V., Semenishin N.N., Korovin Yu.V.
NEW SENSOR POSSIBILITIES OF PORPHYRIN METAL COMPLEXES

Photophysical properties of tetraphenylporphyrine complexes with rare earth ions Lu(III) and Gd(III) in ethanol solutions, polymer films on the basis of polytertbutylmethacrylate and polystyrene and on pressed methocel have been studied. Phosphorescence of complexes in liquid solutions was found out without oxygen. Solid materials doped by complexes were developed; their sensitivity to oxygen at 25 °C was studied.

UDC 544.52+544.526.2+547.587.11+544.142.4

Medyanik N.P., Gureeva N.V., Storozhok N.M., Pozdnyakov I.P.
KINETICS AND MECHANISM OF PHOTOCHEMICAL REACTIONS OF SALICYLIC ACID N-SUBSTITUTED AMIDE

The products of photochemical reactions of 1-(N-4'-hydroxyphenyl-3,3',5'-tritert-butyl)-5-ethyl salicylic acid (I) have been studied by the methods of optical spectroscopy, stationary and nano-second laser pulse photolysis. It is shown by the method of partial molecule deuteration that they are both in unbound state and as complexes with intra- and intermolecule hydrogen bond. Free phenolic groups of amide I are subjected to photolysis that results in formation of phenoxy radicals which extinguish in recombination reactions ($k_{rec} \approx 2{,}3 \cdot 10^8$ l·mole^{-1}·s^{-1}); the formation of radical products due to homolytic decomposition of N-H bond was not established.

UDC 541.64:547.322

Kuchevskaya A.S., Berezina E.M., Filimonova I.L., Ivanov A.A., Filimoshkin A.G.
DYNAMIC OF MICROSTRUCTURE OF MALEIC ANHYDRIDE COPOLYMERS

Prototropic tautomerism occurs in macromolecules of binary maleic anhydride copolymers with vinyl-acetic ester and vinyl chloride and dynamic microstructural nonuniformity consisting of some tautomeric forms: succineanhydride rings, vinyl-chloride, vinyl-acetic units as well as enol (*en*) and dienol (*den*) derivatives of furan (33 mole %) is formed spontaneously. The occurring hydrogen bonds close the ring and form simultaneously the quasi-aromatic structures. Tautomers *en* and *den* form complexes with transformation of charge with O- and N-nucleophiles. The investigations were carried out by the methods of IR-, electron, NMR ^{1}H and ^{13}C spectroscopy, differential thermal analysis, mathematical modeling of microstructure in solution etc.

UDC [547.23+547.29:542.943]:530.145

Potapov A.S., Domina G.A., Khlebnikov A.I., Ogorodnikov V.D., Petrenko T.V.
THEORETICAL AND EXPERIMENTAL RESEARCH OF CARBOXYLATION OF SOME BIS(PYRAZOL-1-YL)ALKANES

Carboxylation of a number of bis(pyrazol-1-yl)alkanes with oxalyl chloride forming dicarbonic acids in position of 4 pyrazole cycles has been studied. It was found out that in the case of bis(pyrazol-1-yl)methane the carboxylation ends at the stage of formation of monocarboxylic acid derivative. It was shown with the help of quantum-chemical calculations within the frames of density functional theory that the second pyrazole cycle is decontaminated under the influence of inductive effect of pyrazole ring with the entered functional group.

UDC 665.7.038:66.011

Konovalov K.B., Nesyn G.V., Manzhay V.N., Polyakova N.M.
COMPARISON OF THE METHODS OF MANUFACTURING DRAG REDUCING OIL ADDITIVES ON THE BASIS OF LABORATORY DATA

The methods of manufacturing drag reducing oil additive of suspended type have been compared on the basis of laboratory data; economic efficiency and engineering attraction of two methods: cryogenic grinding of bulk polymer with its next introduction into suspended medium and polymer sedimentation at the early polymerization stage have been estimated.

UDC 678.743.2

Agafonova A.I., Koval E.O., Mayer E.A.
SELF-EXTINGUISHING COMPOUNDS OF POLYPROPYLENE

The results of investigations of quality indices for self-extinguishing compounds of polypropylene have been introduced. The data on compound incombustibility index developed using inorganic and organic antipyrens containing and not containing halogens are introduced.

UDC 378.662.147.72:54

Minin M.G., Mamontov V.V., Stas N.F.
INTEGRATION OF THE CHAIRS OF TOMSK UNIVERSITIES IN DIDACTIC STUDIES IN CHEMISTRY

Integration of efforts of universities in Tomsk scientific-educational complex for developing objective diagnostics of the quality of students' knowledge in chemistry has been examined. The main stages of works were considered chronologically. The professors contributed most of all to this work were mentioned.